



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 21, 2018 – 11:46 PM EST

PDB ID : 6BK8
EMDB ID: : EMD-7109
Title : S. cerevisiae spliceosomal post-catalytic P complex
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on : 2017-11-07
Resolution : 3.30 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

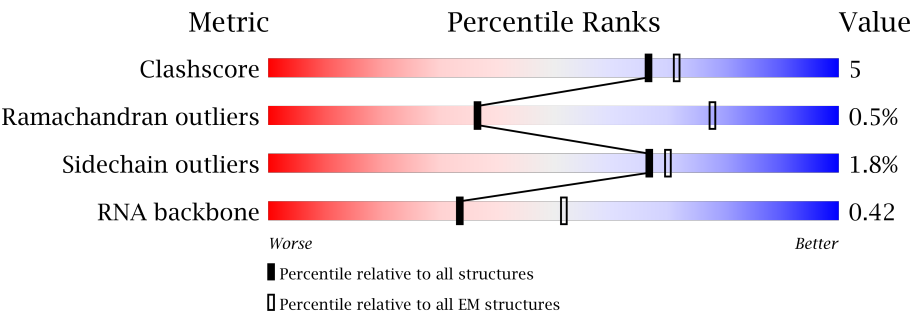
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




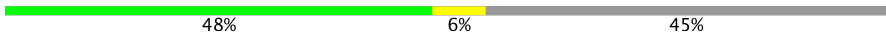














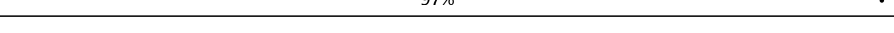
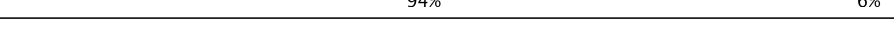







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	1175	<div><div>7% .. 89%</div></div>
2	5	214	<div><div>30% 13% . . 52%</div></div>
3	6	112	<div><div>50% 31% 9% . 9%</div></div>
4	e	34	<div><div>35% 44% 21%</div></div>
5	i	59	<div><div>69% 27% .</div></div>
6	A	2413	<div><div>68% 13% 19%</div></div>
7	B	1008	<div><div>75% 14% . 11%</div></div>
8	D	451	<div><div>65% 14% . 20%</div></div>






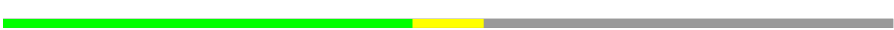






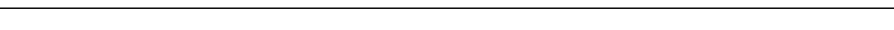
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Mol	Chain	Length	Quality of chain
9	E	379	
10	F	364	
11	G	339	
12	H	175	
13	I	157	
14	K	135	
15	L	577	
16	M	455	
17	N	251	
18	O	382	
19	P	1145	
20	R	215	
21	S	590	
22	T	687	
23	U	859	
24	X	219	
25	Y	16	
26	a	110	
26	q	110	
27	b	86	
27	m	86	
28	c	94	
28	l	94	
29	d	77	
29	n	77	

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Mol	Chain	Length	Quality of chain
30	f	196	 41%59%
30	k	196	 38%60%
31	g	101	 81%19%
31	o	101	 74%23%
32	h	146	 55%44%
32	p	146	 46%8%46%
33	r	111	 76%24%
34	s	238	 66%31%
35	u	503	 85%14%
35	v	503	 22%77%
35	w	503	 86%13%
35	x	503	 23%77%
36	y	175	 59%37%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 82745 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	135	Total	C	N	O	P	0	0
			2848	1272	472	969	135		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	103	Total	C	N	O	P	0	0
			2173	973	367	730	103		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	102	Total	C	N	O	P	0	0
			2170	972	386	710	102		

- Molecule 4 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	34	Total	C	N	O	P	0	0
			707	319	107	247	34		

- Molecule 5 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	i	59	Total	C	N	O	P	0	0
			1239	558	202	420	59		

- Molecule 6 is a protein called Pre-mRNA-splicing factor Prp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1960	Total	C	N	O	S	0	0
			16159	10381	2786	2933	59		

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	899	Total	C	N	O	S	0	0
			7179	4638	1191	1321	29		

- Molecule 8 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	359	Total	C	N	O	S	0	0
			2826	1786	497	533	10		

- Molecule 9 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	186	Total	C	N	O	S	0	0
			1494	939	276	273	6		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	199	Total	C	N	O	S	0	0
			1576	991	277	293	15		

- Molecule 11 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	255	Total	C	N	O	S	0	0
			2048	1297	362	378	11		

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	70	Total	C	N	O	S	0	0
			570	357	113	99	1		

- Molecule 13 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	156	Total	C	N	O	S	0	0
			1283	803	239	231	10		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	82	Total	C	N	O	S	0	0
			550	332	106	111	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	412	Total	C	N	O	S	0	0
			3353	2160	556	620	17		

- Molecule 16 is a protein called Pre-mRNA-processing factor Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	326	Total	C	N	O	S	0	0
			2607	1649	465	485	8		

- Molecule 17 is a protein called Pre-mRNA-splicing factor Prp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	167	Total	C	N	O	S	0	0
			1326	856	233	233	4		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	229	Total	C	N	O	S	0	0
			1935	1211	347	368	9		

- Molecule 19 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	653	Total	C	N	O	S	0	0
			3872	2393	736	740	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	101	Total	C	N	O	S	0	0
			813	499	150	163	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	238	Total	C	N	O	S	0	0
			1948	1218	355	368	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	483	Total	C	N	O	S	0	0
			3370	2113	624	625	8		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	637	Total	C	N	O	S	0	0
			3625	2226	689	703	7		

- Molecule 24 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	219	Total	C	N	O	0	0
			1095	657	219	219		

- Molecule 25 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
26	q	93	Total	C	N	O	S	0	0
			726	468	136	118	4		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
27	m	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
28	l	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
29	n	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
30	k	78	Total	C	N	O	S	0	0
			610	389	109	109	3		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
31	o	78	Total	C	N	O	S	0	0
			600	384	104	110	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
32	p	79	Total	C	N	O	S	0	0
			618	393	107	116	2		

- Molecule 33 is a protein called Lea1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	r	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 34 is a protein called Msl1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 35 is a protein called Pre-mRNA-processing factor Prp19.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	u	435	Total	C	N	O	0	0
			2156	1286	435	435		
35	v	118	Total	C	N	O	0	0
			588	352	118	118		
35	w	438	Total	C	N	O	0	0
			2171	1295	438	438		
35	x	116	Total	C	N	O	0	0
			578	346	116	116		

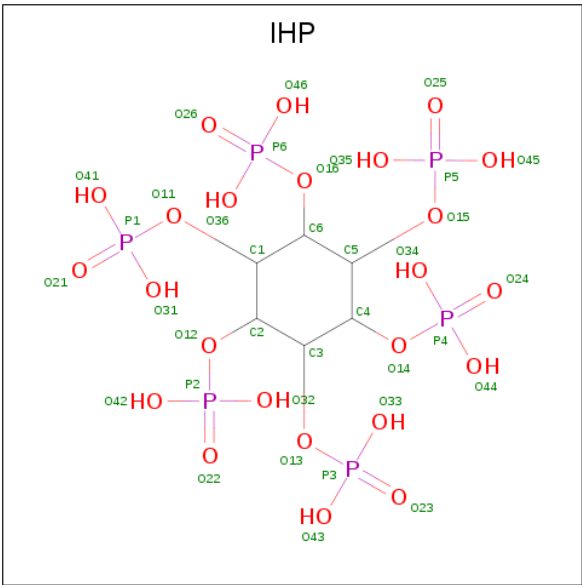
- Molecule 36 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	y	110	Total	C	N	O	0	0
			548	328	110	110		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

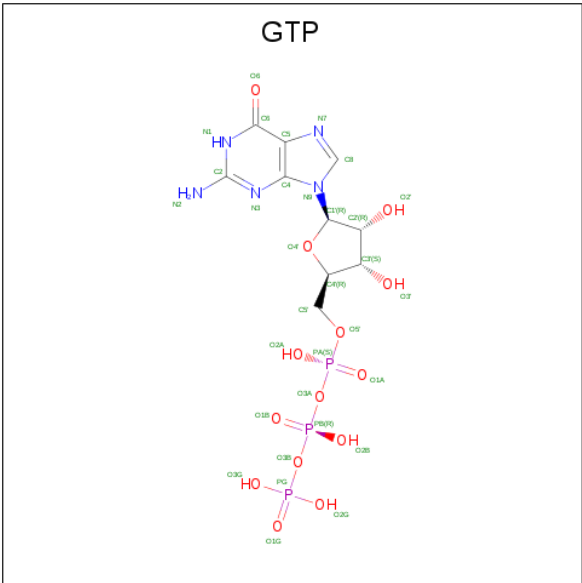
Mol	Chain	Residues	Atoms		AltConf
37	B	1	Total	Mg	0
			1	1	
37	6	4	Total	Mg	0
			4	4	

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

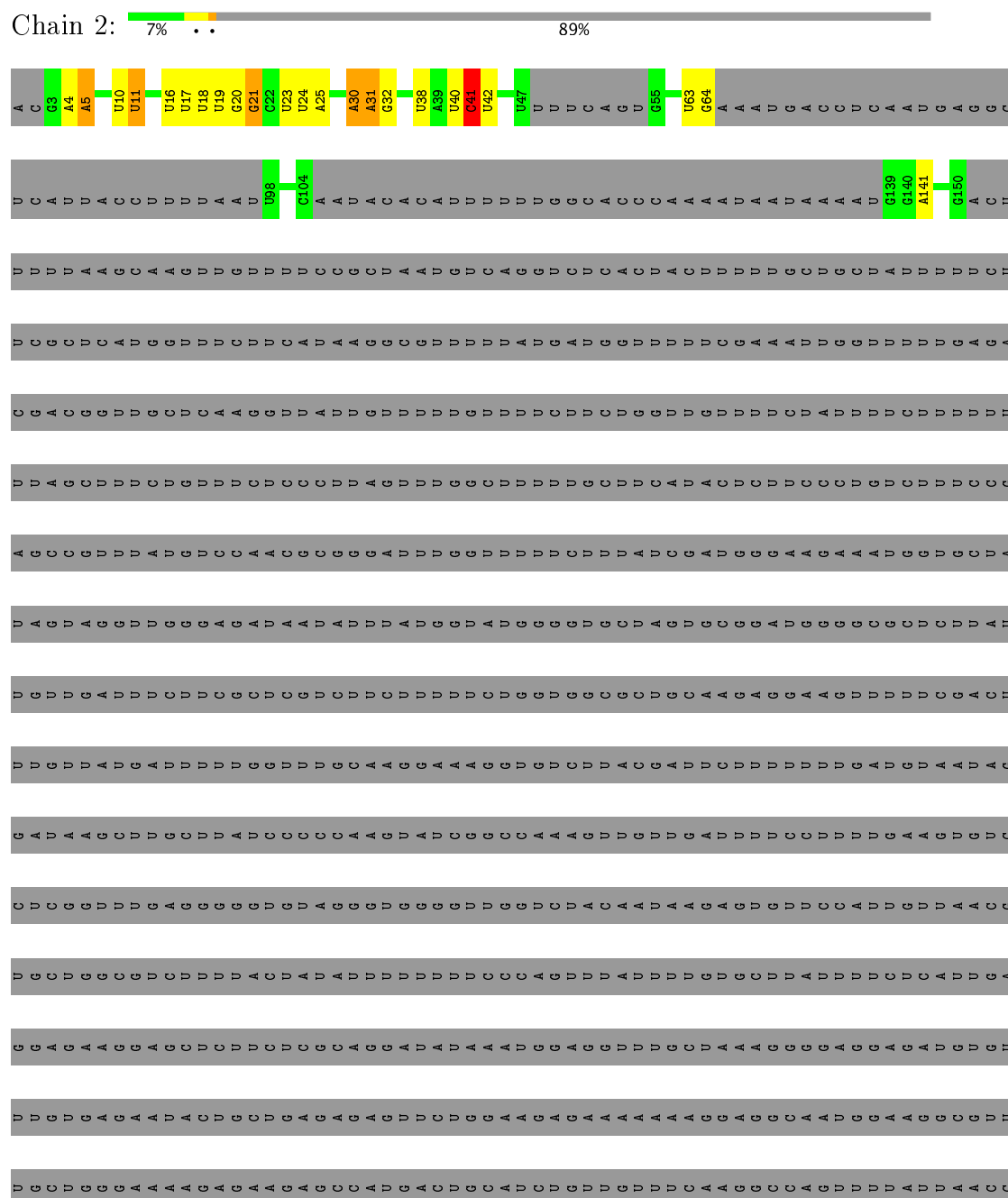
- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	G	1	Total 1	Zn 1	0
40	I	3	Total 3	Zn 3	0
40	F	2	Total 2	Zn 2	0
40	O	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

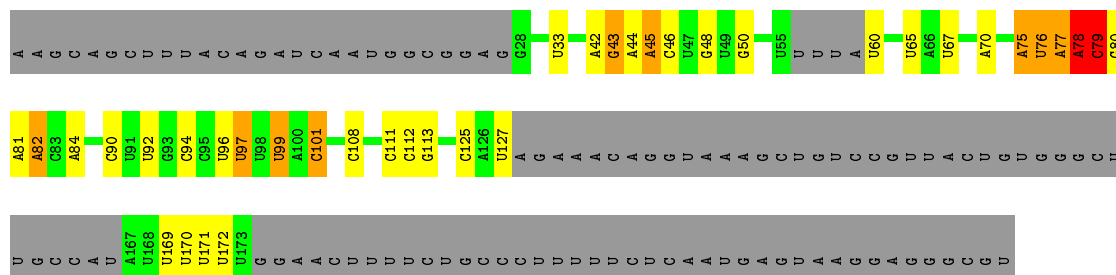
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: U2 snRNA



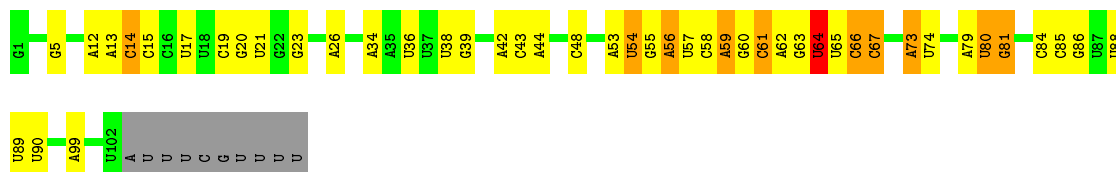
- Molecule 2: U5 snRNA

Chain 5:  30% 13% . . 52%



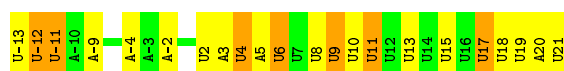
- Molecule 3: U6 snRNA

Chain 6:  50% 31% 9% 9%



- Molecule 4: RNA (34-MER)

Chain e:  35% 44% 21%



- Molecule 5: RNA (59-MER)

Chain i:  69% 27% .



- Molecule 6: Pre-mRNA-splicing factor Prp8

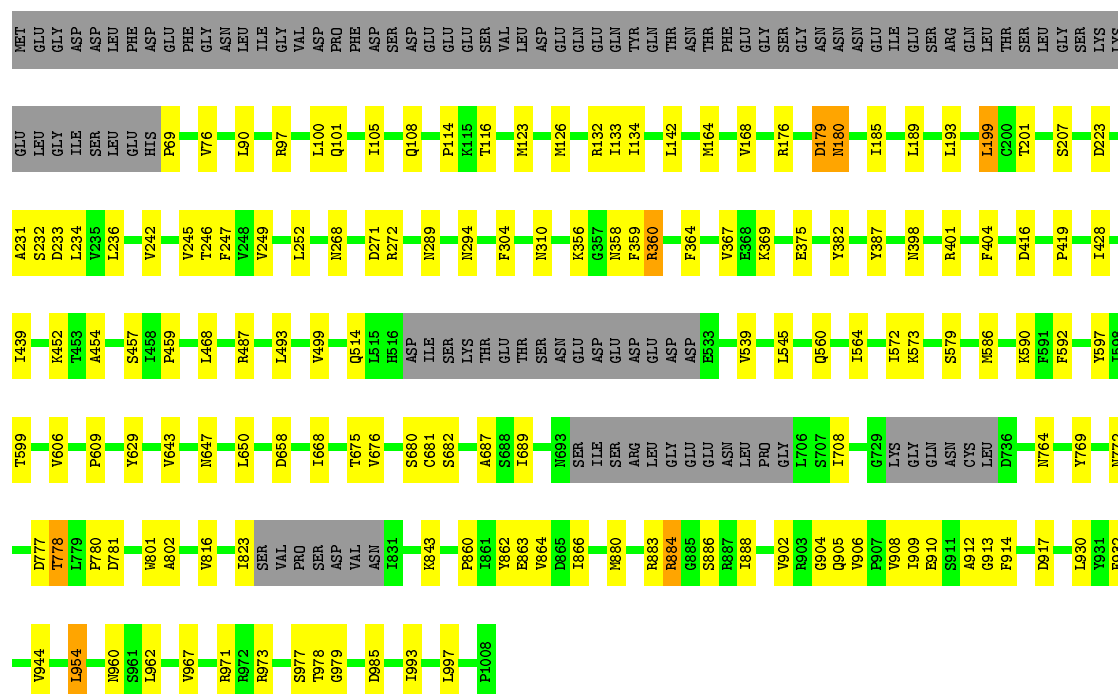
Chain A:  68% 13% 19%



[illegible]

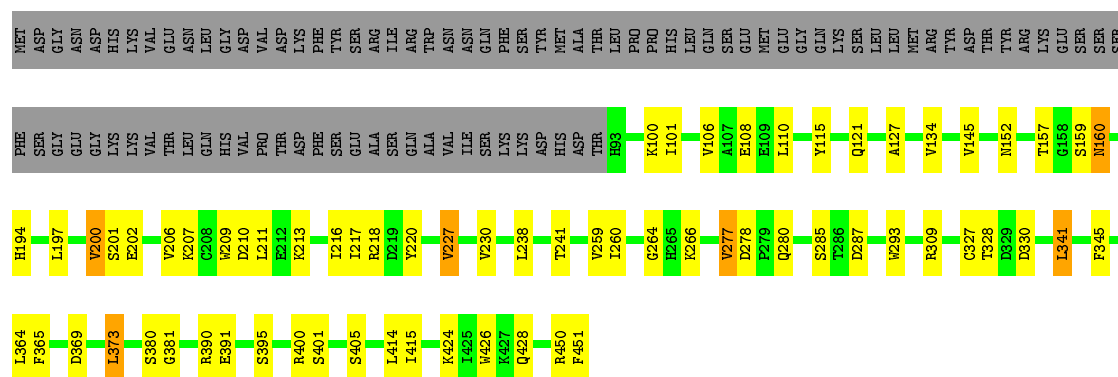
- Molecule 7: Pre-mRNA-splicing factor SNU114

Chain B:  75% 14% 11%



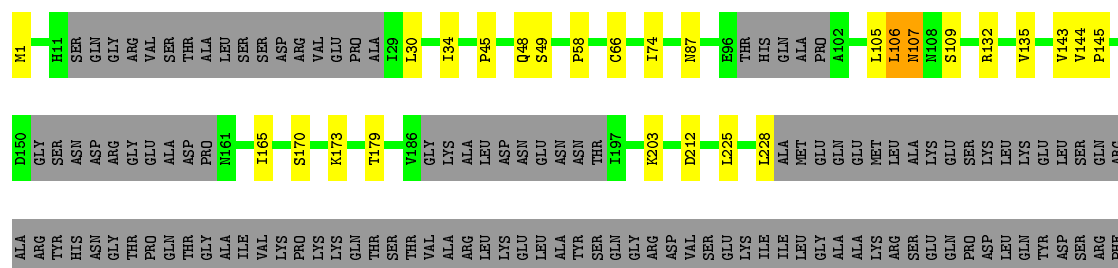
• Molecule 8: Pre-mRNA-splicing factor PRP46

Chain D:  65% 14% 20%



• Molecule 9: Pre-mRNA-processing protein 45

Chain E:  42% 7% 51%



PHE THR ARG THR GLY ALA ASN ALA ALA SER SER LYS ARG HIS GLU GLN ASP ASN PRO LEU PHE VAL GLN GLN ASP ILE GLU SER ILE TYR LYS THR ASN TYR TYR GLU LYS ASP ASP ALA VAL VAL ASN VAL LYS SER SER GLY GLY ALA ALA SER GLY HIS GLY PRO PRO ILE GLN PHE THR LYS

ALA
GLU
SER
ASP
ASP
LYS
SER
ASP
ASN
TYR
GLY
ALA

- Molecule 10: Pre-mRNA-splicing factor SLT11

Chain F:  48% 6% 45%

[illegible]

ALA	LEU	TRP	TRP	ASN	GLU	LYS	GLY	ALA	ASN	ASN	GLU	VAL	LYS	VAL	LEU	LEU	GLU	TRP	ALA	SER	SER	VAL	ASP	ILE	ILE	SER	HIS	ILE	LEU	LEU	LEU	ASN	GLU	GLU	GLU	ASP	PHE	LYS	LYS	LYS	ASN	ASN	PRO	PRO	SER	SER	THR	K203	I214	K218	L227	GLY	ILE	GLY	LYS	LYS	TRP	ASP	ASP	GLY	ASN	SER	LEU	K230
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[illegible]

GLY	LEU	SER	PHE	PRO	THR	LYS	SER	THR	ASP	ASN	ALA	LYS	ASN	ASP	LYS	LYS	LYS	THR	SER	LYS	LYS	VAL	HIS	LYS	ASP	ARG	SER	LYS	LYS	SER	LYS	PRO	ARG	ALA	ASN	LYS	LEU	THR	ILE
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- Molecule 11: Pre-mRNA-splicing factor CWC2

Chain G: 66% 7% 25%

MET	THR	S3	P19	P23	W37	M44	P55	C81	H91	H2	I93	D98	L102	T106	L109	G113	D119	Y120	R121	V139	A145	L151	K152	P153	R159	Y175	V176	K179	L206	P207	W212	R215	L221	P257	R257
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ASN	SER	ALA	GLY	THR	GLU	VAL	ASN	ASN	LYS	ASN	ASN	GLU	ARG	LEU	ARG	ASP	ARG	THR	PHE	PRO	GLU	ALA	SER	SER	VAL	ASP	ASN	VAL	LYS	LYS	ARG	LEU	LEU	PRO	PRO	LEU	LEU	GLY	GLY	ASN	ASP	ASP	PHE	TLE	ILE	GLU	GLU	LYS	LYS	LEU	LEU	LYS	LYS	VAL	LYS	LYS	LYS	ASN	ASN	TLE	SER	ARG	GLU	GLU	ASN	TLE	SER	PER
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ASP
GLU
ASP

- Molecule 12: Pre-mRNA-splicing factor CWC15

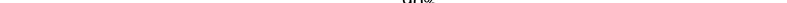
Chain H:  32% 6% 60%

MET	T2	T3	R6	P7	L8	O8	E10	L30	H34	T35	T36	K41	PHE	LYS	GLU	GLU	GLU	GLU	GLU	ASN	ASN	ASP	CYS	GLN	ASP	ASP	ASP	LYS	LYS	SER	LEU	LEU	GLU	GLU	GLU	ALA	VAL	MET	MET	ASN	ASN	GLU	GLU	GLU	GLU	LYS	GLN	ASP	ASP	VAL	VAL	GLY	GLY	SER	SER	ASN	ASN	LEU	LEU	GLN	GLN	GLU	GLU	THR
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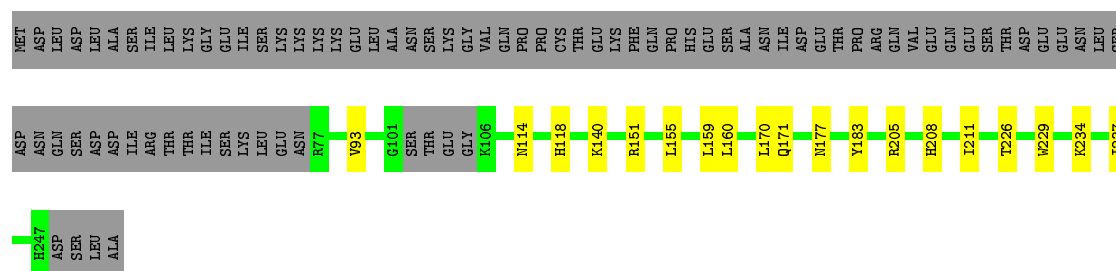
[illegible]

SER
ALA
SER
GLY
Y156
I157
N158
L170
H173
V174
R175

- Molecule 13: Pre-mRNA-splicing factor BUD31

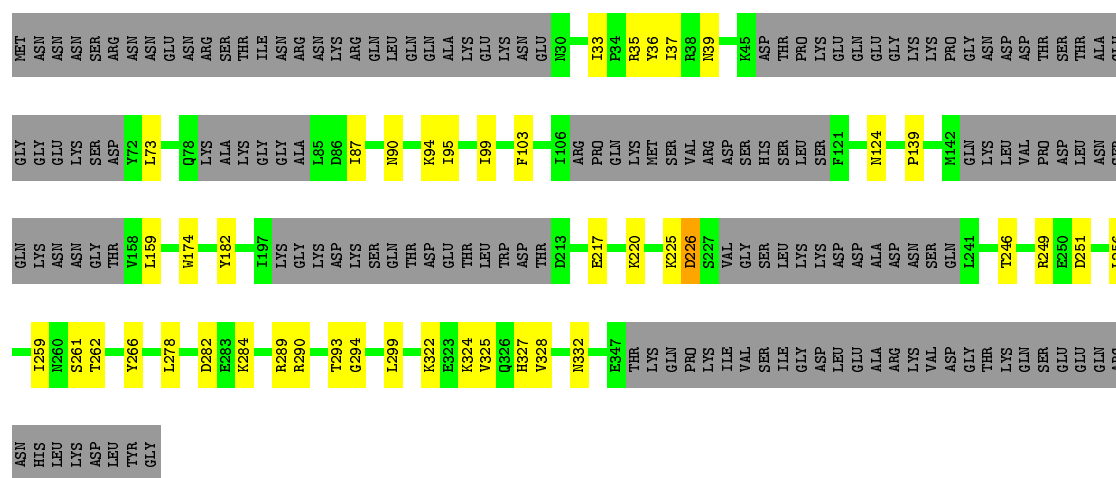
Chain I:  90% 9%

Chain N:  59% 8% 33%



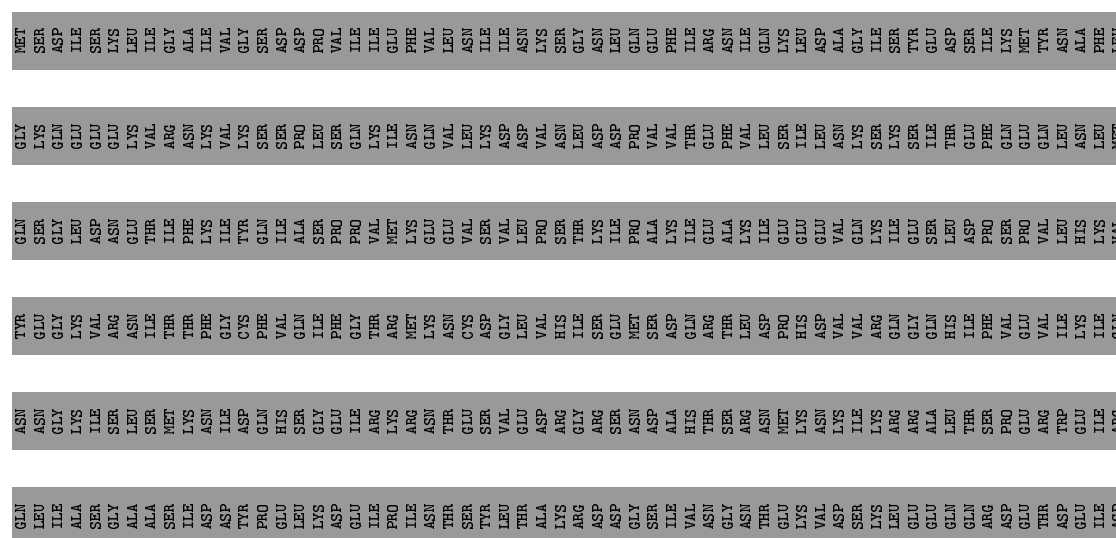
- Molecule 18: Pre-mRNA-splicing factor SLU7

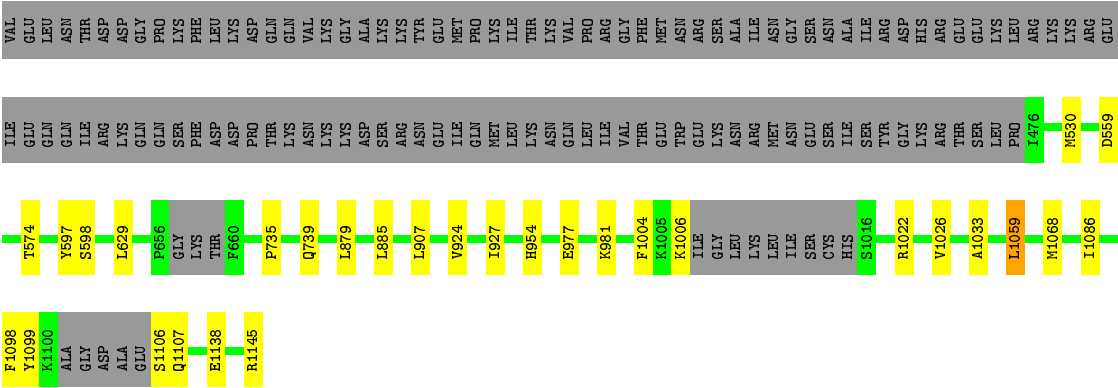
Chain O:  49% 11% 40%



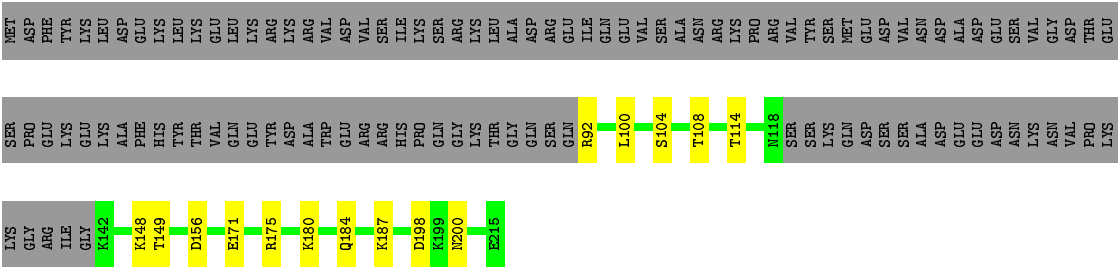
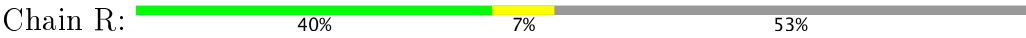
- Molecule 19: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22

Chain P: 54% . 43%

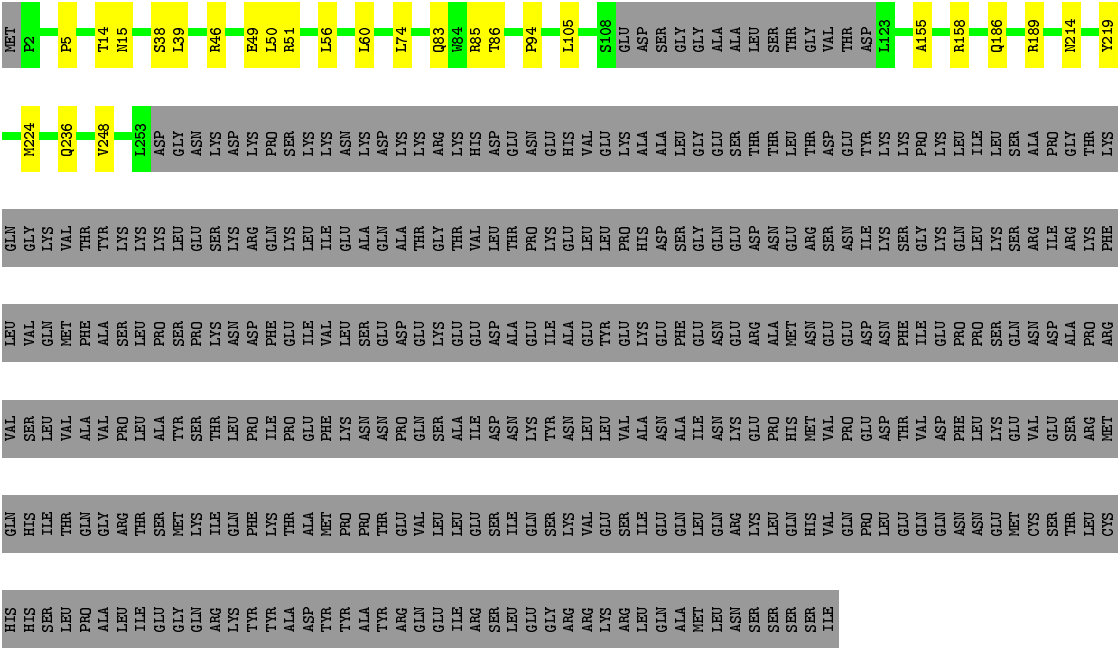




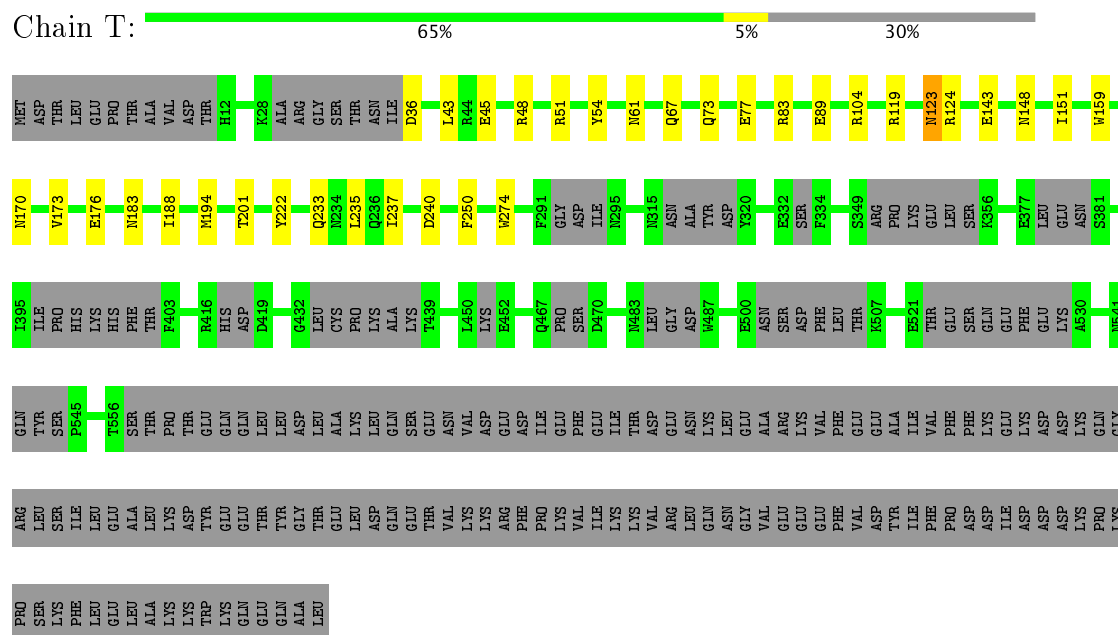
• Molecule 20: Pre-mRNA-splicing factor SYF2



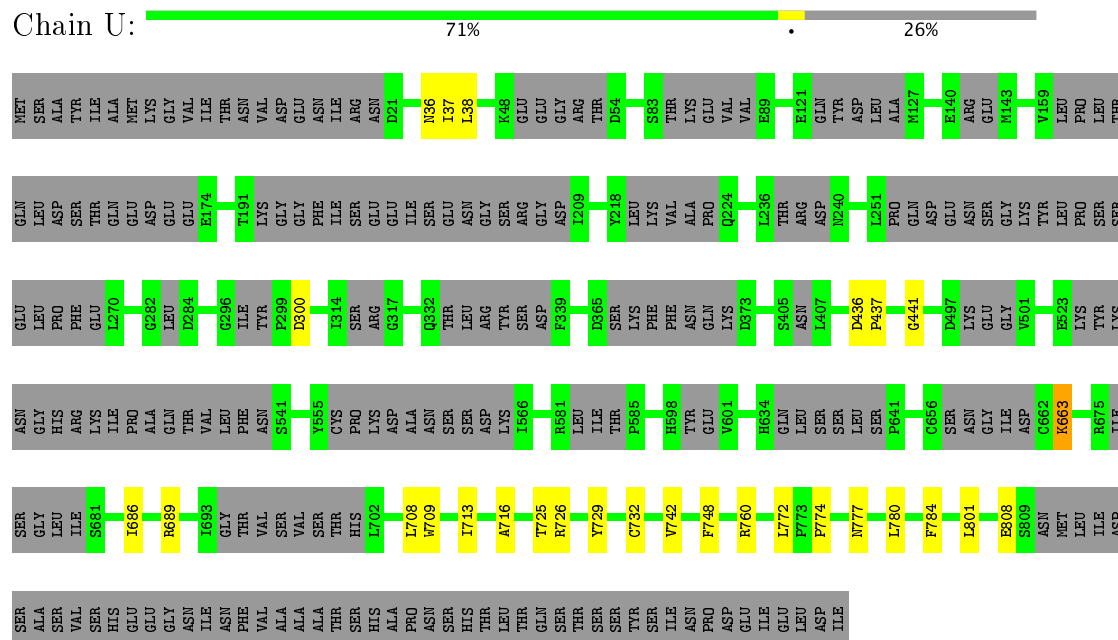
• Molecule 21: Pre-mRNA-splicing factor CEF1



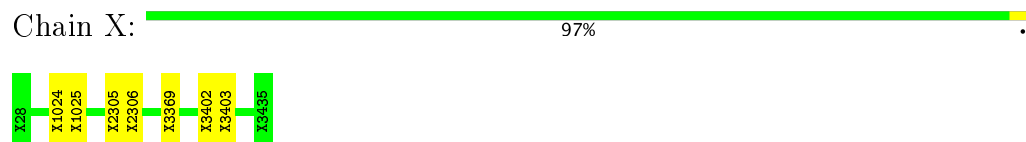
• Molecule 22: Pre-mRNA-splicing factor CLF1



• Molecule 23: Pre-mRNA-splicing factor SYF1



• Molecule 24: Unknown protein fragment




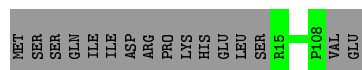
• Molecule 25: Unknown protein fragment

Chain Y:  94% 6%




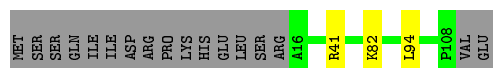
- Molecule 26: Small nuclear ribonucleoprotein Sm D2

Chain a:  85% 15%




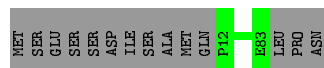
- Molecule 26: Small nuclear ribonucleoprotein Sm D2

Chain q:  82% 15%




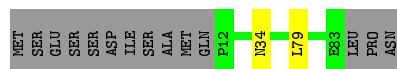
- Molecule 27: Small nuclear ribonucleoprotein F

Chain b:  84% 16%




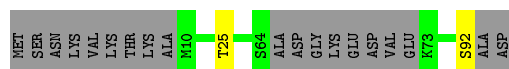
- Molecule 27: Small nuclear ribonucleoprotein F

Chain m:  81% 16%



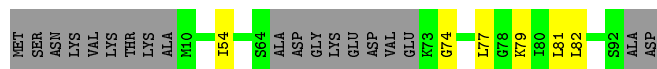
- Molecule 28: Small nuclear ribonucleoprotein E

Chain c:  78% 20%




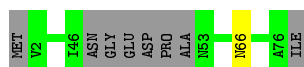
- Molecule 28: Small nuclear ribonucleoprotein E

Chain l:  73% 6% 20%

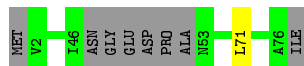
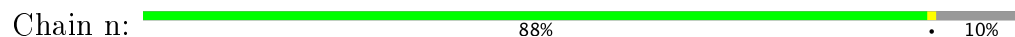


- Molecule 29: Small nuclear ribonucleoprotein G

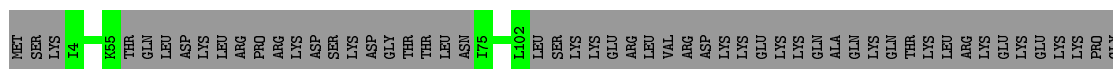
Chain d:  88% 10%



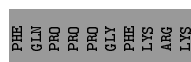
- Molecule 29: Small nuclear ribonucleoprotein G



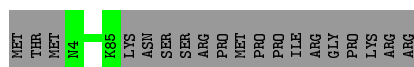
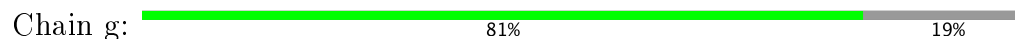
- Molecule 30: Small nuclear ribonucleoprotein-associated protein B



- Molecule 30: Small nuclear ribonucleoprotein-associated protein B



- Molecule 31: Small nuclear ribonucleoprotein Sm D3

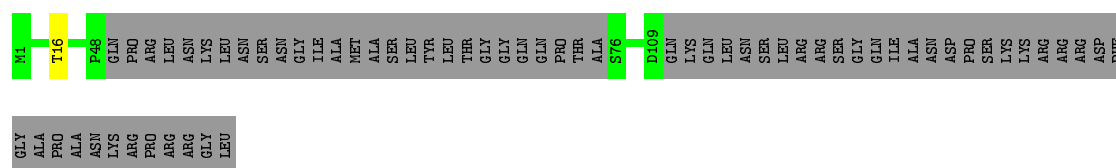


- Molecule 31: Small nuclear ribonucleoprotein Sm D3



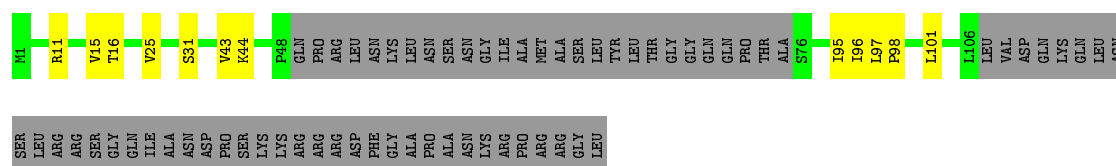
- Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain h:  55% . 44%



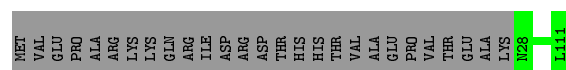
- Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain p: 



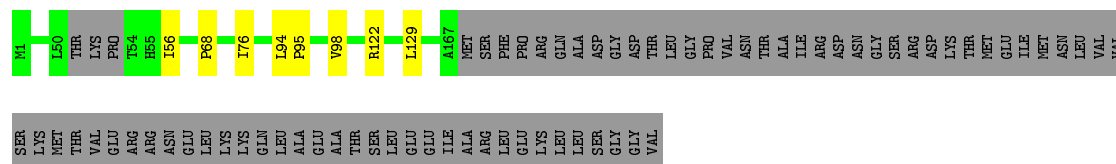
- Molecule 33: Lea1

Chain r:  76% 24%



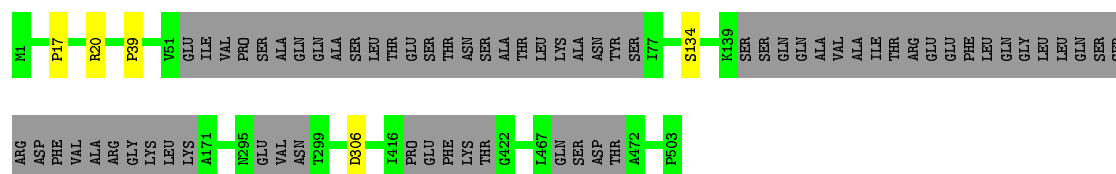
- Molecule 34: Msl1

Chain s: 66% . 31%



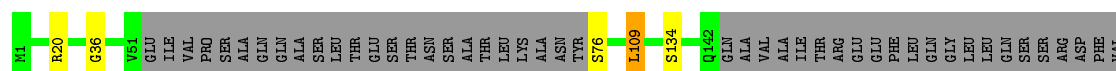
- Molecule 35: Pre-mRNA-processing factor Prp19

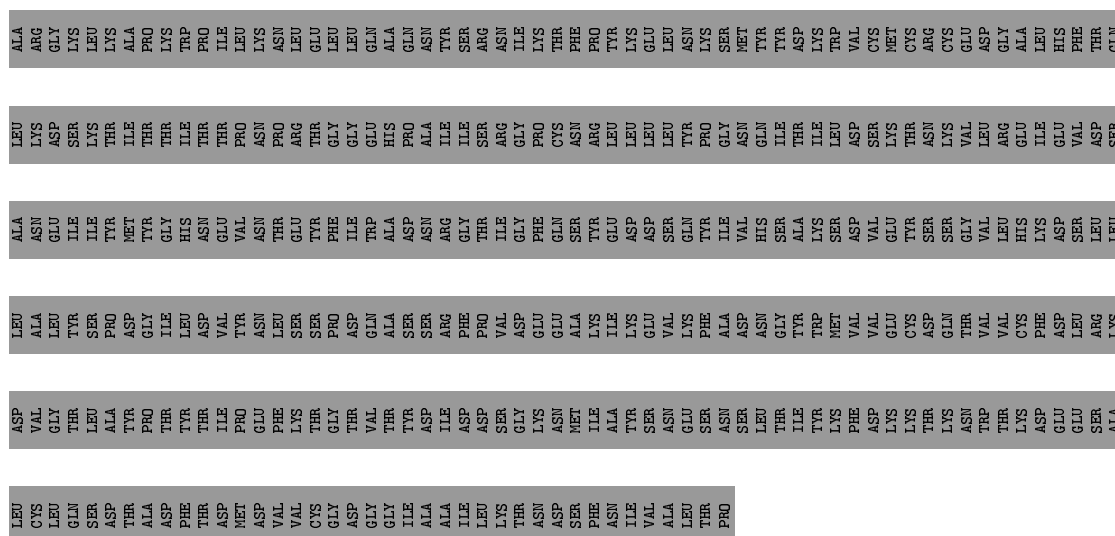
Chain u: 85% • 14%



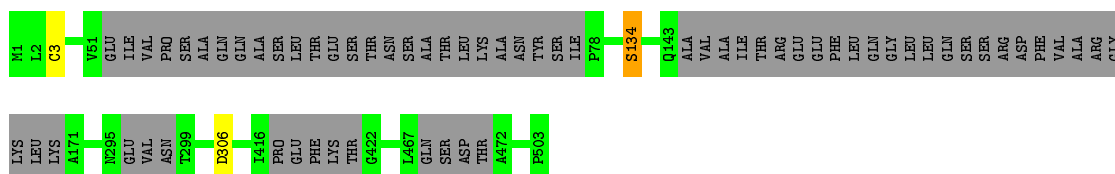
- Molecule 35: Pre-mRNA-processing factor Prp19

Chain v: 22% 77%

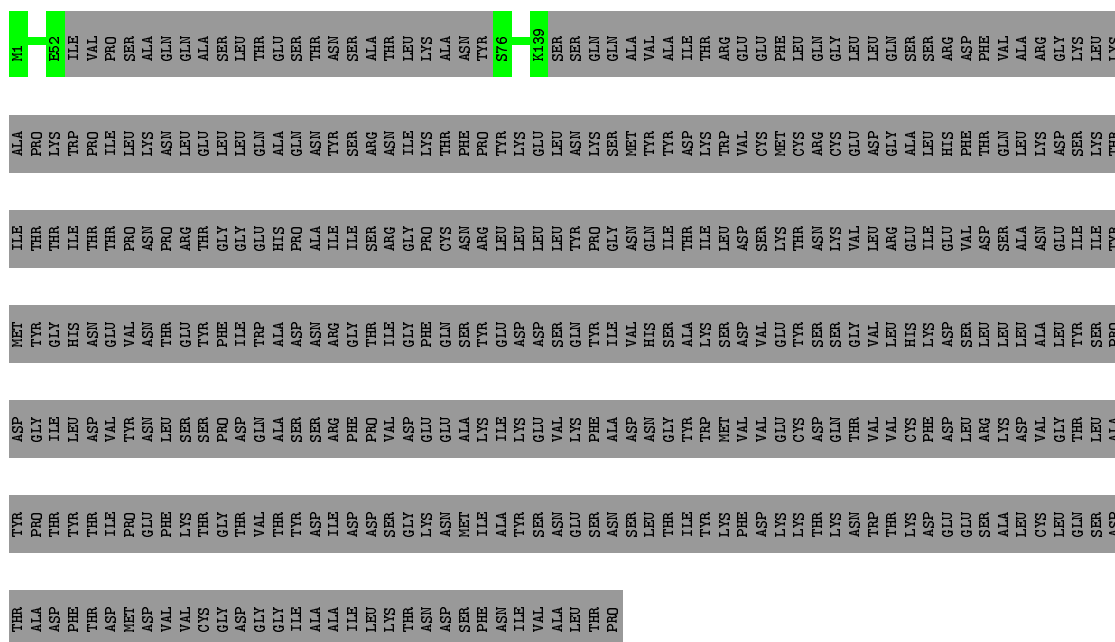




- Molecule 35: Pre-mRNA-processing factor Prp19



- Molecule 35: Pre-mRNA-processing factor Prp19



- Molecule 36: Pre-mRNA-splicing factor SNT309

Chain y:



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212219	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, IHP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	2	0.50	1/3167 (0.0%)	0.92	8/4911 (0.2%)
10	F	0.43	0/1598	0.67	2/2151 (0.1%)
11	G	0.47	0/2094	0.62	2/2815 (0.1%)
12	H	0.41	0/584	0.76	1/781 (0.1%)
13	I	0.49	0/1307	0.59	0/1748
14	K	0.35	0/552	0.56	0/746
15	L	0.38	0/3406	0.63	1/4592 (0.0%)
16	M	0.37	0/2678	0.61	1/3619 (0.0%)
17	N	0.39	0/1354	0.59	0/1838
18	O	0.36	0/1967	0.62	2/2624 (0.1%)
19	P	0.29	0/3918	0.48	2/5386 (0.0%)
2	5	0.88	0/2422	1.16	21/3762 (0.6%)
20	R	0.39	0/817	0.57	1/1083 (0.1%)
21	S	0.46	0/1978	0.63	1/2655 (0.0%)
22	T	0.45	0/3411	0.55	1/4632 (0.0%)
23	U	0.27	0/3625	0.45	0/4963
26	a	0.36	0/753	0.57	0/1013
26	q	0.38	0/738	0.61	0/995
27	b	0.41	0/585	0.57	0/791
27	m	0.40	0/585	0.61	0/791
28	c	0.42	0/585	0.61	0/795
28	l	0.40	0/585	0.56	0/795
29	d	0.50	0/532	0.61	0/715
29	n	0.36	0/529	0.50	0/711
3	6	0.89	0/2427	1.13	15/3778 (0.4%)
30	f	0.36	0/636	0.63	0/856
30	k	0.35	0/614	0.57	0/826
31	g	0.35	0/634	0.56	0/859
31	o	0.37	0/607	0.53	0/820
32	h	0.38	0/649	0.54	0/880
32	p	0.40	0/623	0.65	0/844
33	r	0.33	0/415	0.55	0/577

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
34	s	0.31	0/814	0.53	0/1134
35	u	0.47	0/2150	0.68	2/2989 (0.1%)
35	v	0.59	0/586	0.89	3/816 (0.4%)
35	w	0.47	0/2165	0.71	3/3010 (0.1%)
35	x	0.58	0/576	0.79	0/802
36	y	0.58	0/546	0.80	0/760
4	e	0.82	4/787 (0.5%)	1.48	17/1219 (1.4%)
5	i	0.59	0/1379	1.10	3/2131 (0.1%)
6	A	0.52	0/16570	0.68	8/22456 (0.0%)
7	B	0.49	0/7331	0.70	8/9926 (0.1%)
8	D	0.56	1/2889 (0.0%)	0.71	2/3924 (0.1%)
9	E	0.44	0/1517	0.63	0/2043
All	All	0.49	6/83685 (0.0%)	0.72	104/115562 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	F	0	1
11	G	0	2
15	L	0	1
18	O	0	1
30	k	0	1
35	u	0	1
35	v	0	1
35	w	0	2
36	y	0	2
6	A	0	6
7	B	0	9
8	D	0	2
9	E	0	3
All	All	0	32

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	9	U	C1'-N1	7.04	1.59	1.48
4	e	-13	U	C1'-N1	6.81	1.58	1.48
4	e	-11	U	C1'-N1	6.04	1.57	1.48
4	e	-2	A	N9-C4	-6.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	227	VAL	CB-CG1	-5.37	1.41	1.52

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	954	LEU	CA-CB-CG	9.20	136.46	115.30
4	e	11	U	C2-N1-C1'	9.14	128.67	117.70
4	e	11	U	N1-C2-O2	8.22	128.55	122.80
35	w	134	SER	CA-C-O	-7.91	103.49	120.10
4	e	2	U	N1-C2-O2	7.86	128.30	122.80

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	405	ASN	Peptide
6	A	542	HIS	Peptide
6	A	774	ILE	Peptide
6	A	775	ARG	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2848	0	1445	11	0
2	5	2173	0	1102	11	0
3	6	2170	0	1095	14	0
4	e	707	0	354	0	0
5	i	1239	0	624	0	0
6	A	16159	0	16162	181	0
7	B	7179	0	7361	76	0
8	D	2826	0	2816	47	0
9	E	1494	0	1540	22	0
10	F	1576	0	1607	13	0
11	G	2048	0	2011	17	0
12	H	570	0	556	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	I	1283	0	1301	10	0
14	K	550	0	454	2	0
15	L	3353	0	3421	30	0
16	M	2607	0	2512	41	0
17	N	1326	0	1367	13	0
18	O	1935	0	1894	35	0
19	P	3872	0	2618	16	0
20	R	813	0	837	11	0
21	S	1948	0	1979	20	0
22	T	3370	0	2727	22	0
23	U	3625	0	2248	15	0
24	X	1095	0	231	9	0
25	Y	80	0	18	1	0
26	a	741	0	778	0	0
26	q	726	0	754	0	0
27	b	573	0	572	0	0
27	m	573	0	572	0	0
28	c	575	0	597	0	0
28	l	575	0	597	0	0
29	d	529	0	557	0	0
29	n	526	0	555	0	0
30	f	631	0	670	0	0
30	k	610	0	638	0	0
31	g	625	0	647	0	0
31	o	600	0	623	0	0
32	h	644	0	686	0	0
32	p	618	0	660	0	0
33	r	416	0	182	0	0
34	s	816	0	341	0	0
35	u	2156	0	938	0	0
35	v	588	0	250	0	0
35	w	2171	0	945	0	0
35	x	578	0	246	0	0
36	y	548	0	219	0	0
37	6	4	0	0	0	0
37	B	1	0	0	0	0
38	A	36	0	6	3	0
39	B	32	0	12	0	0
40	F	2	0	0	0	0
40	G	1	0	0	0	0
40	I	3	0	0	0	0
40	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	82745	0	70325	520	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 520 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:212:ASP:OD2	24:X:1024:UNK:O	1.57	1.22
13:I:150:CYS:SG	13:I:153:CYS:HB3	2.11	0.90
19:P:598:SER:O	19:P:629:LEU:HA	1.75	0.87
1:2:1108:A:N6	20:R:108:THR:CB	107.65	0.84
11:G:81:CYS:SG	11:G:91:HIS:HE1	2.01	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	1954/2413 (81%)	1813 (93%)	126 (6%)	15 (1%)	22	57
7	B	889/1008 (88%)	830 (93%)	55 (6%)	4 (0%)	38	71
8	D	357/451 (79%)	329 (92%)	28 (8%)	0	100	100
9	E	176/379 (46%)	164 (93%)	11 (6%)	1 (1%)	28	63
10	F	193/364 (53%)	173 (90%)	19 (10%)	1 (0%)	32	66
11	G	253/339 (75%)	229 (90%)	23 (9%)	1 (0%)	38	71
12	H	64/175 (37%)	55 (86%)	8 (12%)	1 (2%)	11	43
13	I	154/157 (98%)	140 (91%)	14 (9%)	0	100	100
14	K	76/135 (56%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	L	406/577 (70%)	380 (94%)	26 (6%)	0	100	100
16	M	320/455 (70%)	302 (94%)	18 (6%)	0	100	100
17	N	163/251 (65%)	157 (96%)	6 (4%)	0	100	100
18	O	215/382 (56%)	196 (91%)	19 (9%)	0	100	100
19	P	645/1145 (56%)	610 (95%)	35 (5%)	0	100	100
20	R	97/215 (45%)	94 (97%)	3 (3%)	0	100	100
21	S	234/590 (40%)	223 (95%)	11 (5%)	0	100	100
22	T	451/687 (66%)	442 (98%)	9 (2%)	0	100	100
23	U	587/859 (68%)	555 (94%)	30 (5%)	2 (0%)	44	76
26	a	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
26	q	91/110 (83%)	84 (92%)	7 (8%)	0	100	100
27	b	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	m	70/86 (81%)	65 (93%)	5 (7%)	0	100	100
28	c	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
28	l	71/94 (76%)	66 (93%)	4 (6%)	1 (1%)	13	46
29	d	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
29	n	65/77 (84%)	57 (88%)	8 (12%)	0	100	100
30	f	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
30	k	74/196 (38%)	66 (89%)	7 (10%)	1 (1%)	13	46
31	g	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
31	o	74/101 (73%)	70 (95%)	4 (5%)	0	100	100
32	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
32	p	75/146 (51%)	65 (87%)	8 (11%)	2 (3%)	6	32
33	r	82/111 (74%)	76 (93%)	6 (7%)	0	100	100
34	s	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	2	17
35	u	423/503 (84%)	413 (98%)	8 (2%)	2 (0%)	32	66
35	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	6	33
35	w	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
35	x	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
36	y	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	2	14
All	All	9709/14738 (66%)	9051 (93%)	610 (6%)	48 (0%)	37	66

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	1905	LEU
12	H	9	LEU
23	U	37	ILE
34	s	76	ILE
36	y	94	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	1778/2182 (82%)	1741 (98%)	37 (2%)	59	81
7	B	809/910 (89%)	797 (98%)	12 (2%)	70	85
8	D	313/397 (79%)	307 (98%)	6 (2%)	62	81
9	E	168/328 (51%)	166 (99%)	2 (1%)	75	87
10	F	183/332 (55%)	183 (100%)	0	100	100
11	G	219/296 (74%)	216 (99%)	3 (1%)	71	85
12	H	58/151 (38%)	53 (91%)	5 (9%)	12	42
13	I	140/141 (99%)	139 (99%)	1 (1%)	87	92
14	K	44/121 (36%)	43 (98%)	1 (2%)	56	79
15	L	379/538 (70%)	377 (100%)	2 (0%)	91	94
16	M	288/413 (70%)	283 (98%)	5 (2%)	66	83
17	N	144/225 (64%)	143 (99%)	1 (1%)	87	92
18	O	210/346 (61%)	208 (99%)	2 (1%)	80	88
19	P	178/1029 (17%)	176 (99%)	2 (1%)	78	88
20	R	90/193 (47%)	89 (99%)	1 (1%)	78	88
21	S	208/525 (40%)	207 (100%)	1 (0%)	91	94
22	T	248/633 (39%)	244 (98%)	4 (2%)	68	84
23	U	131/786 (17%)	126 (96%)	5 (4%)	38	70
26	a	79/103 (77%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	q	77/103 (75%)	74 (96%)	3 (4%)	37	70
27	b	63/77 (82%)	63 (100%)	0	100	100
27	m	63/77 (82%)	61 (97%)	2 (3%)	44	74
28	c	65/83 (78%)	63 (97%)	2 (3%)	45	75
28	l	65/83 (78%)	60 (92%)	5 (8%)	15	47
29	d	58/66 (88%)	57 (98%)	1 (2%)	66	83
29	n	57/66 (86%)	56 (98%)	1 (2%)	64	83
30	f	70/176 (40%)	70 (100%)	0	100	100
30	k	67/176 (38%)	66 (98%)	1 (2%)	70	85
31	g	69/89 (78%)	69 (100%)	0	100	100
31	o	67/89 (75%)	64 (96%)	3 (4%)	32	67
32	h	77/129 (60%)	76 (99%)	1 (1%)	73	86
32	p	73/129 (57%)	63 (86%)	10 (14%)	4	20
All	All	6538/10992 (60%)	6419 (98%)	119 (2%)	67	83

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	D	227	VAL
14	K	71	ARG
32	p	25	VAL
9	E	87	ASN
12	H	8	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
7	B	1004	ASN
12	H	8	GLN
23	U	777	ASN
8	D	428	GLN
10	F	89	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	127/1175 (10%)	44 (34%)	4 (3%)
2	5	100/214 (46%)	25 (25%)	2 (2%)
3	6	101/112 (90%)	28 (27%)	3 (2%)
4	e	33/34 (97%)	19 (57%)	0
5	i	54/59 (91%)	18 (33%)	0
All	All	415/1594 (26%)	134 (32%)	9 (2%)

5 of 134 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	11	U
1	2	16	U
1	2	17	U
1	2	18	U

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	78	A
3	6	64	U
3	6	14	C
1	2	1124	U
2	5	81	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
38	IHP	A	3001	-	36,36,36	0.83	0	54,60,60	1.53	8 (14%)
39	GTP	B	2001	37	27,34,34	1.12	2 (7%)	27,54,54	1.93	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	IHP	A	3001	-	-	0/30/54/54	0/1/1/1
39	GTP	B	2001	37	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	2001	GTP	O4'-C4'	-2.11	1.40	1.45
39	B	2001	GTP	C6-N1	2.46	1.37	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B	2001	GTP	N3-C2-N1	-5.44	119.52	127.46
39	B	2001	GTP	C1'-N9-C4	-3.49	120.60	126.64
39	B	2001	GTP	C6-C5-C4	-2.81	118.05	120.84
39	B	2001	GTP	N2-C2-N1	2.13	120.64	117.24
38	A	3001	IHP	O15-C5-C4	2.30	114.11	108.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A	3001	IHP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	X	4
5	i	4

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	15:U	O3'	501:A	P	58.05
1	X	3370:UNK	C	3389:UNK	N	35.33
1	X	1031:UNK	C	2287:UNK	N	34.77
1	X	125:UNK	C	1001:UNK	N	25.13
1	X	2322:UNK	C	3364:UNK	N	19.85